# 5F-EDMB-PICA

<table>
<thead>
<tr>
<th>Sample Type:</th>
<th>Seized Material</th>
</tr>
</thead>
<tbody>
<tr>
<td>Latest Revision:</td>
<td>December 3, 2020</td>
</tr>
<tr>
<td>Date Received:</td>
<td>July 24, 2020</td>
</tr>
<tr>
<td>Date of Report:</td>
<td>December 3, 2020</td>
</tr>
</tbody>
</table>

## 1. GENERAL INFORMATION

<table>
<thead>
<tr>
<th>IUPAC Name:</th>
<th>Ethyl 2-[[1-(5-fluoropentyl)indole-3-carbonyl]amino]-3,3-dimethyl-butanoate</th>
</tr>
</thead>
<tbody>
<tr>
<td>InChI String:</td>
<td>InChI=1S/C22H31FN2O3/c1-5-28-21(27)19(22(2,3)4)24-20(26)17-15-25(14-10-6-9-13-23)18-12-8-7-11-16(17)18/h7-8,11-12,15,19H,5-6,9-10,13-14H2,1-4H3,(H,24,26)</td>
</tr>
<tr>
<td>CFR:</td>
<td>Not Scheduled (12/2020)</td>
</tr>
<tr>
<td>CAS#:</td>
<td>Not Available</td>
</tr>
<tr>
<td>Synonyms:</td>
<td>5-fluoro EDMB-PICA, 5F-EDMB-2201, 5-fluoro EDMB-2201</td>
</tr>
<tr>
<td>Source:</td>
<td>NMS Labs – Criminalistic Laboratory</td>
</tr>
<tr>
<td>Appearance:</td>
<td>Plant-Like Material</td>
</tr>
</tbody>
</table>

**Important Note**: All identifications were made based on evaluation of analytical data (GC-MS and LC-QTOF-MS) in comparison to analysis of acquired reference material.

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### 2. CHEMICAL AND PHYSICAL DATA

#### 2.1 CHEMICAL DATA

<table>
<thead>
<tr>
<th>Form</th>
<th>Chemical Formula</th>
<th>Molecular Weight</th>
<th>Molecular Ion [M⁺]</th>
<th>Exact Mass [M+H]⁺</th>
</tr>
</thead>
<tbody>
<tr>
<td>Base</td>
<td>C₂₂H₃₁FN₅O₃</td>
<td>390.5</td>
<td>390</td>
<td>391.2391</td>
</tr>
</tbody>
</table>

#### 3. BRIEF DESCRIPTION

5F-EDMB-PICA is classified as a synthetic cannabinoid. Synthetic cannabinoids have been reported to cause psychoactive effects similar to delta-9-tetrahydrocannabinol (THC). Synthetic cannabinoids have caused adverse events, including deaths, as described in the literature. 5F-MDMB-PICA and 5F-EDMB-PINACA are structurally similar synthetic cannabinoids. 5F-MDMB-PICA was first reported by NPS Discovery in July 2018 and 5F-EDMB-PINACA was first reported by NPS Discovery in April 2018. 5F-MDMB-PICA and 5F-EDMB-PINACA are Schedule I substances in the United States; 5F-EDMB-PICA is not explicitly scheduled.

#### 4. ADDITIONAL RESOURCES

- [https://www.policija.si/apps/nfl_response_web/0_Analytical_Reports_final/5F-EDMB-PICA-ID-HIFS-024_report.pdf](https://www.policija.si/apps/nfl_response_web/0_Analytical_Reports_final/5F-EDMB-PICA-ID-HIFS-024_report.pdf)
- [https://www.policija.si/apps/nfl_response_web/0_Analytical_Reports_final/5F-EDMB-PICA-ID-2191-20_report.pdf](https://www.policija.si/apps/nfl_response_web/0_Analytical_Reports_final/5F-EDMB-PICA-ID-2191-20_report.pdf)
5. QUALITATIVE DATA

5.1 GAS CHROMATOGRAPHY MASS SPECTROMETRY (GC-MS)

Testing Performed At: NMS Labs (Willow Grove, PA)

Sample Preparation: Acid/Base extraction

Instrument: Agilent 5975 Series GC/MSD System

Column: Zebron™ Inferno™ ZB-35HT (15 m x 250 µm x 0.25 µm)

Carrier Gas: Helium (Flow: 1 mL/min)

Temperatures: Injection Port: 265 °C

Transfer Line: 300 °C

MS Source: 230 °C

MS Quad: 150 °C

Oven Program: 60 °C for 0.5 min, 35 °C/min to 340 °C for 6.5 min

Injection Parameters: Injection Type: Splitless

Injection Volume: 1 µL

MS Parameters: Mass Scan Range: 40-550 m/z

Threshold: 250

Retention Time: 8.24 min

Standard Comparison: Reference material for 5F-EDMB-PICA (Batch: 0588529-1) was purchased from Cayman Chemical (Ann Arbor, MI, USA).

Analysis of this standard resulted in positive identification of the analyte in the exhibit as 5F-EDMB-PICA based on retention time (8.23 min) and mass spectral data.

(https://www.caymanchem.com/product/30725/5-fluoro-edmb-pica)
Chromatogram: 5F-EDMB-PICA

Additional peak present in chromatogram: internal standard (6.32 min)
EI (70 eV) Mass Spectrum (Top) and 10x (Bottom): 5F-EDMB-PICA
5.2 LIQUID CHROMATOGRAPHY QUADRUPOLE TIME OF FLIGHT MASS SPECTROMETRY (LC-QTOF)

Testing Performed At: The Center for Forensic Science Research and Education at the Fredric Rieders Family Foundation (Willow Grove, PA)

Sample Preparation: 1:100 dilution of acid/base extraction in mobile phase

Instrument: Sciex TripleTOF® 5600+, Shimadzu Nexera XR UHPLC

Column: Phenomenex® Kinetex C18 (50 mm x 3.0 mm, 2.6 µm)

Mobile Phase:
A: Ammonium formate (10 mM, pH 3.0)
B: Methanol/acetonitrile (50:50)

Flow rate: 0.4 mL/min

Gradient: Initial: 95A:5B; 5A:95B over 13 min; 95A:5B at 15.5 min

Temperatures:
Autosampler: 15 ºC
Column Oven: 30 ºC
Source Heater: 600 ºC

Injection Parameters:
Injection Volume: 10 µL

QTOF Parameters:
TOF MS Scan Range: 100-510 Da
Precursor Isolation: SWATH® acquisition (27 windows)
Fragmentation: Collison Energy Spread (35±15 eV)
MS/MS Scan Range: 50-510 Da

Retention Time: 9.65 min

Standard Comparison: Reference material for 5F-EDMB-PICA (Batch: 0588529-1) was purchased from Cayman Chemical (Ann Arbor, MI, USA). Analysis of this standard resulted in positive identification of the analyte in the exhibit as 5F-EDMB-PICA based on retention time (9.67 min) and mass spectral data. (https://www.caymanchem.com/product/30725/5-fluoro-edmb-pica)
Chromatogram: 5F-EDMB-PICA

Additional peak present in chromatogram: internal standard (7.31 min)
TOF MS (Top) and MS/MS (Bottom) Spectra: 5F-EDMB-PICA